Three-Dimensional Quantum Transport by Supercell Method: Numerical Acceleration and Applications

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Abstract. The open-boundary planar supercell stack method treats three-dimensional quantum transport in mesoscopic tunnel structures in a numerically stable and efficient manner. The method formulates quantum mechanical scattering problems for the supercell geometry as sparse linear systems, which can be solved by iterative methods. Recent improvement in solution algorithm using a seven-diagonal pre-conditioner has resulted in over two orders of magnitude of numerical acceleration, bringing more flexibility in the range of problems we can tackle. We will discuss applications to interface roughness in double barrier resonant tunneling structures and tunneling characteristics of ultra-thin oxides undergoing dielectric breakdown.

1. Introduction

The exactly solvable, real-space, open-boundary planar supercell stack method (OPSSM) has been applied to a variety of topics involving three-dimensional quantum transport in mesoscopic devices [1]. The method was designed for studying elastic scattering effects due to impurities, interface roughness, and alloy disorder in our studies of 2D (double barrier heterostructures), 1D (quantum wires electron wave guides), and 0D (quantum dots) mesoscopic device structures. OPSSM studies have demonstrated: interfacial inhomogeneities in double barrier resonant tunneling diodes can induce lateral localization of wave functions [2], strongly attractive impurities can produce additional transmission

resonance [3], clustering effects in alloy barriers can reduce barrier effectiveness, and surface roughness in quantum dots can cause large fluctuations in transmission characteristics [4]. In addition, OPSSM has also been used to study resonant tunneling via self-organized quantum dot states [5], and interface roughness effects [6] and dielectric breakdown [7] in n^+ poly-Si/SiO_2/p-Si tunnel structures containing ultra-thin oxide layers. In this paper, we present the results of our recent work on numerical acceleration. These new implementations have led to up to two orders of magnitude gains in computational efficiency, greatly extending the range of applicability of OPSSM.

2. Method

The generic device structure treated by OPSSM consists of a slab of active region sandwiched between two semi-infinite, homogeneous, flat-band electrode regions. The active region is described by a stack of planar supercells which can take on quasi-3D variations. Let the z axis be the direction of current flow. Then the active region is composed of a stack of N_Z layers perpendicular to the z-direction, with each layer containing a periodic array of rectangular planar supercells of N_X by N_Y sites. Within each planar supercell, the potential assumes lateral variations as dictated by device geometry. A one-band nearest-neighbor tight-binding Hamiltonian is used to describe the potential and effective mass variations over this volume of interest [1].

OPSSM formulates quantum mechanical scattering problems for supercell geometries as a complex, non-Hermitian, sparse linear system $\boldsymbol{A}x=b$. Here $\boldsymbol{A}$ is the Hamiltonian matrix, augmented by special terms representing opening boundary conditions; x is a vector containing the coefficients of the tight-binding orbitals (which is equivalent to the envelope function in the effective mass approximation); and b is a vector describing the open boundary condition [1]. As the order of the linear system (N_X x N_Y x N_Z) can be quite large, direct solution methods are impractical for all but the smallest supercells. However, the linear system can be solved iteratively using the Quasi-Minimal Residual (QMR) method [8], which is capable of treating non-Hermitian systems. As with other iterative methods, the convergence behavior and efficiency of QMR depends on the eigenvalue spectrum of $\boldsymbol{A}$. In some cases QMR may not work or may converge too slowly to be practical. These problems can be greatly ameliorated by employing a good pre-conditioner [8]. The idea is to use a pre-conditioning matrix $\boldsymbol{M}$ to transform the original problem into an equivalent one $(\boldsymbol{M}^{-1}\boldsymbol{A})x=\boldsymbol{M}^{-1}b$. The pre-conditioner $\boldsymbol{M}$ should be easily invertable, and should approximate $\boldsymbol{A}$ is some sense. (Note that if $\boldsymbol{M}=\boldsymbol{A}$, the problem is solved.) For good choices of $\boldsymbol{M}$, the transformed problem can be solved in significantly fewer iterations than the original one. In general, there are no set rules for constructing good pre-conditioners. In this work, we present the results from the application of a seven-diagonal pre-conditioner [9] which appears to be well-suited to our system.

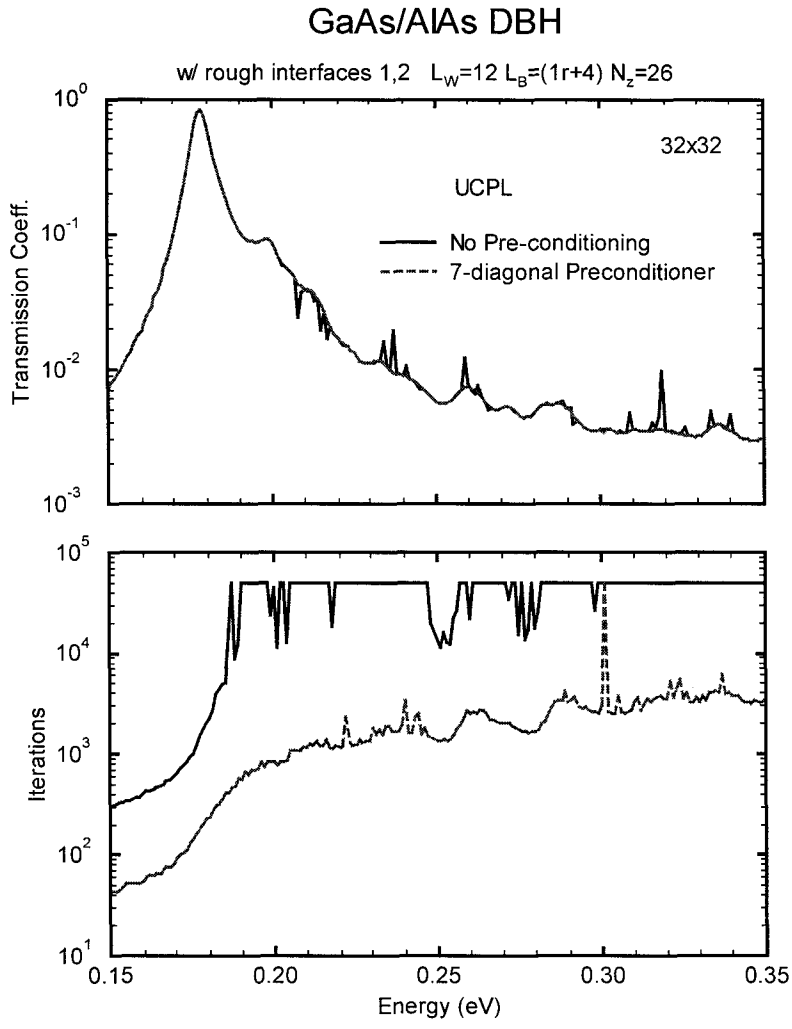

Figure 1 Upper panel shows transmission coefficient spectra of GaAs/AlAs double barrier structure. Lower panel shows convergence iterations counts with and without the 7-diagonal pre-conditioner. A limit of 50,000 iteration is used.

3. Results and Discussions

Fig. 1 illustrate the performance gains achieved using a 7-diagonal pre-conditioner in typical applications involving the studies of interface roughness effects in GaAs/AlAs double barrier resonant tunneling heterostructures [2]. The supercell stack consists of N_Z=26 layers, and the size of the planer supercell is 32x32. We plot the computed transmission coefficient and the number of iterations required for reaching convergence over an energy range of interest, using both non-pre-conditioned and pre-conditioned algorithms. A cutoff of 50,000 iterations is imposed to the total run time. In general, we find that the number of iterations required to reach convergence increases with increasing incoming electron energy, or decreasing deBroglie wavelength. Without pre-conditioning, approximate 30 out of 200 points in the spectrum fail to converge within 50,000 iterations. The application of the 7-diagonal pre-conditioner substantially reduces the number of iterations required to reach

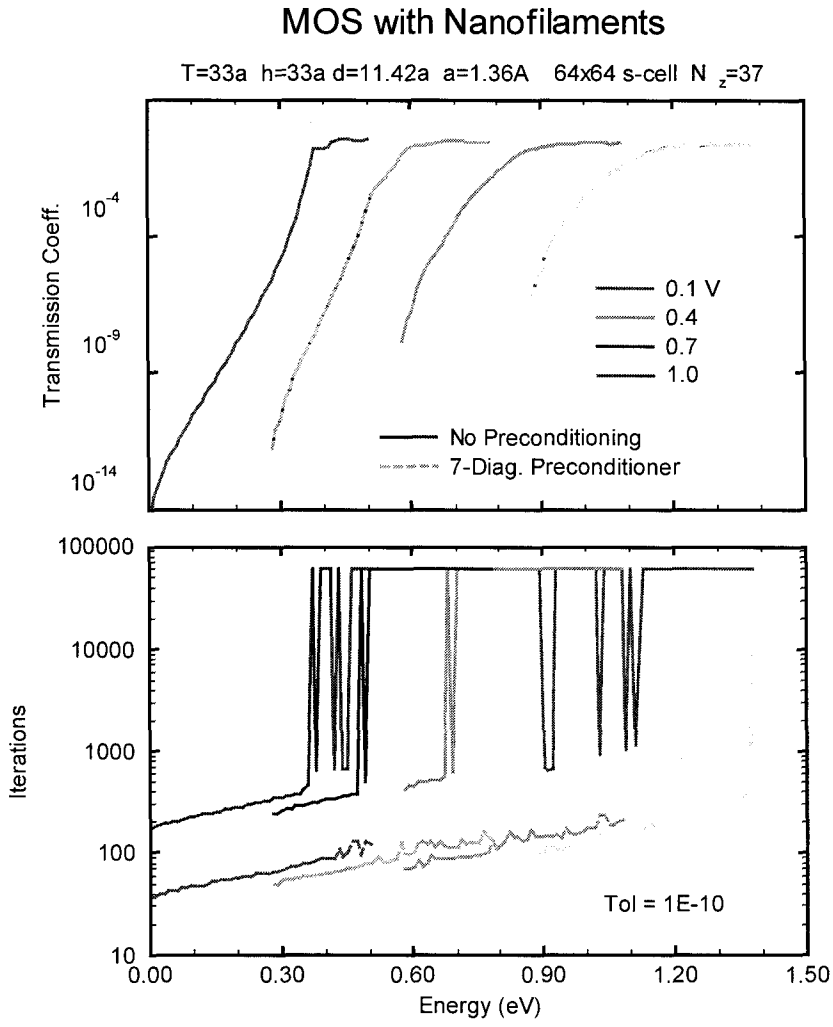

Figure 2 Upper panel shows transmission coefficient spectra of an ultra-thin oxide layer embedded with nano-filaments under several biasing conditions. Lower panel shows convergence iterations counts with and without the 7-diagonal pre-conditioner.

convergence. As a result, only 1 out of 200 points in the spectrum did not converge. Fig. 2 shows application to the study of ultra-thin oxide tunnel structures with embedded nano-filaments as a model of dielectric breakdown [7]. The supercell stack consists of N_Z=37 layers of 64x64 planer supercells. In this case, convergence was reach within the limit of 60,000 iterations for all cases. However, without pre-conditioning, more than half of points required 60,000 iterations. With pre-conditioning, all except for 2 points converged in fewer than 400 iterations. Table 1 summarizes the timing results for some typical applications, and documents the degree of numerical acceleration resulting from the application of the 7-diagonal pre-conditioner. The combination of a suitable pre-conditioner and a more judicious choice of convergence tolerance has resulted in almost a 300-fold speed-up in large supercell applications.

With over two orders of magnitude of numerical acceleration, we are now able to obtain more accurate results by using larger supercells. Previously, calculations of interface

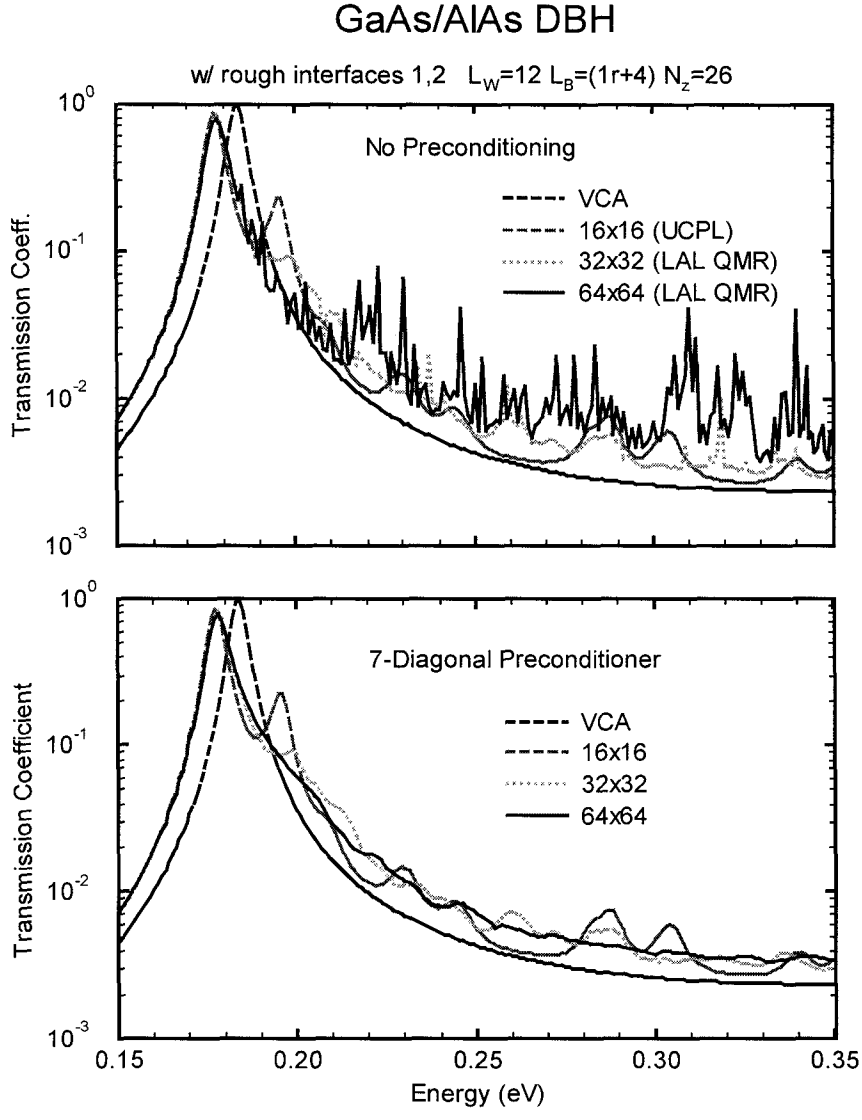

Figure 3 Transmission coefficient spectra of GaAs/AlAs double barrier structure computed using various supercell sizes. Numerical acceleration by pre-conditioning made large supercell calculations possible, thus enabling the reduction of artifacts due to supercell-periodic scattering.

roughness effects on resonant tunneling properties of double barrier heterostructures were performed using modestly sized (20x20 or 32x32) planar supercells [2, 10]. The resulting transmission spectra always contained satellite peaks above the main resonance. While these satellite peaks were very useful in clarifying the interface roughness assisted resonant tunneling mechanism, they are also identified as artifacts induced by the periodic boundary condition associated with the finite supercell [2]. Reference [2] suggested that the use of larger supercells could suppress these artifacts. However, previous attempts plagued by convergence problems. The top panel of Fig. 3 shows transmission coefficients calculated using three different planar supercell sizes (16x16, 32x32, and 64x64) without pre-conditioning. The 64x64 results are not usable due to lack of convergence. The bottom panel shows calculations performed with pre-conditioning. The finite supercell artifacts in

Table 1. Speed-up obtained in typical 3D scattering calculations with a 7-diagonal pre-conditioner.

	No Pre-conditioner	7-Diagonal Preconditioner	Speed-Up
DBH 16x16x26	8.92 h	1.66 h	5.4
DBH 32x32x26	208.7 h	17.6 h	12
DBH 64x64x26	1511 h (Poor Convergence)	283.2 h (Good Convergence)	>> 5
MOS 64x64x37 (Tol=1E-10)	1618.5 h	23.2 h	70
MOS 64x64x37	1618.5 h (Tol=1E-10)	5.7 h (Tol=1E-7)	284

the 16x16 and 32x32 results have essentially disappeared from the 64x64 result. In addition, computation time was greatly reduced.

In summary, we demonstrated over two orders of magnitude of numerical acceleration in our solution algorithm of 3D quantum mechanical scattering code by using a seven-diagonal pre-conditioner. The improvement brings more flexibility in the range of quantum device modeling problems we can tackle.

Acknowledgement

JNS acknowledges support from the Defense Advanced Research Projects Agency (N00014-98-C-0325). DZT acknowledge support from DARPA through the Jet Propulsion Laboratory Technology Affiliates Program with HRL Laboratories. MG acknowledges support from HRL Laboratories and the State of California under a MICRO grant (UC MICRO 99-050).

References

[1] Ting D Z-Y 1999 *Microelectronics J.* **30** 985-1000
[2] Ting D Z-Y, Kirby S K and McGill T C 1994 *Appl. Phys. Lett.* **64** 2004-6
[3] Kirby S K, Ting D Z-Y and McGill T C 1993 *Phys. Rev. B* **48** 15237-44
[4] Kirby S K, Ting D Z-Y and McGill T C 1994 *Semicond. Sci. Tech.* **9** *Suppl.* **S** 918-21
[5] Wang J N, Li R G, Wang Y Q, Ge W K, Ting D Z-Y 1998 *Microelectron Eng* **43-4** 341-47
[6] Ting D Z-Y 1998 *Appl. Phys. Lett.* **73** 2769-7
[7] Ting D Z-Y 1999 *Appl. Phys. Lett.* **74** 585-7
[8] Freund R W, Nachtigal N M 1991 *Numer. Math.* **60** 315-39; 1996 *ACM T Math Software* **22** 46-77
[9] Cao J W, unpublished.
[10] Ting D Z-Y and McGill T C 1996 *J Vac Sci Technol B* **14** 2790-3